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Mills College



OAKLAND 13, CALIFORNIA

February 23, 1965

Professor Joshua Lederberg
Stanford University School of Medicine
Palo Alto, California

Dear Professor Lederberg:

Thank you very much indeed for sending me the copy of your Jan. 18 letter to Dr. Hunsberger, your kind words about our NRC "Survey of Chemical Notation Systems," and the copy of your "Dendral 64" report. I have studied this with much interest and shall look forward to receiving the further parts when they are printed.

As I'm sure you realize, an alphabetic index of the acyclic Dendral notations that you cite would bring together structures with a formal mathematical relationship, but which are not chemically related in terms of the functional groups present. In my opinion the Wiswesser notation is a superior chemical indexing tool since its initial symbols give indexing prominence to the functional groups in acyclic notations.

However, for cyclic structures, your mathematical treatment may well offer valuable insights. My colleagues and I, who are undertaking the revision of the Wiswesser notation, as described in the NRC "Survey", have only recently found a mathematical basis for some of our cyclic notation rules, which we are revising accordingly. I shall therefore be particularly interested in learning more about your treatment of cyclic structures in your Dendral notation.

As a rather minor point, may I point out that the second and third Wiswesser notations you cite in Table 5 are quite incorrect. They perhaps illustrate Mr. Hayward's lack of knowledge about the Wiswesser notation, but it seems a pity to disseminate this misinformation further. Our statement in the "Survey" that these notations were incorrect was unfortunately deleted. You will find an authentic comparison of the Hayward, IUPAC and Wiswesser notations on page 55 of the NRC "Survey."

I appreciate your sending me the Dendral 64 paper and I hope you will send the further parts of the report as they are printed.

Sincerely,

Elbert G. Smith

Elbert G. Smith
Professor of Chemistry